AD-A139 262 A NEW METHOD FOR OBTAINING INDIVIDUAL COMPONENT SPECTRA FROM THOSE OF COM..(U) INDIANA UNIV AT BLOOMINGTON DEPT OF CHEMISTRY D E HONIGS ET AL. 10 MAR 84 1/1

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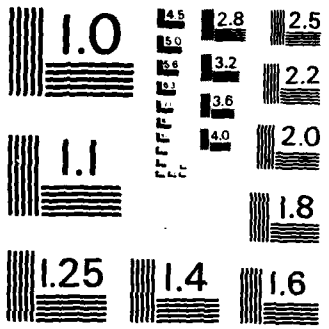

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20. Abstract - continued...

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OFFICE OF NAVAL RESEARCH

Contract N14-76-C-0838

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A NEW METHOD FOR OBTAINING INDIVIDUAL COMPONENT SPECTRA FROM THOSE OF COMPLEX MIXTURES

by

D. E. HONIGS AND G. M. HIEFTJE

Prepared for Publication

in

APPLIED SPECTROSCOPY

Indiana University
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Bloomington, Indiana 47405

10 March 1984

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ABSTRACT

In Near-Infrared Reflectance Analysis (NIRA), a computer is trained to recognize and quantitate the relationship between the near-infrared spectrum of a sample and the concentrations of one or more of the sample constituents. During this training process the computer implicitly generates the spectrum of the constituents in question although this spectrum is ordinarily not available for operator inspection. In the present study, a method for displaying this implicit information is developed and evaluated. The resulting "reconstructed spectrum" can be of a specific chemical constituent in a sample or can be a composite spectrum of those components that collectively contribute to specific sample properties such as material strength, processing temperature or to sensory characteristics such as the "hotness" of peppers. A comparison is made of this new spectral reconstruction technique to established methods such as spectral stripping and factor analysis.

INTRODUCTION

Near-infrared reflectance analysis (NIRA) methods operate by using a set of samples of known composition whose spectra are employed as a "training set" for a multilinear regression algorithm.[1-4] A computer then selects a set of wavelengths and generates weighting coefficients whose application to unknown sample spectra then predicts their composition.

This technique has been applied with tremendous success to extremely difficult samples, in which almost complete spectral overlap obscured individual bands and where no band was interference-free, where background fluctuations far exceeded spectral changes caused by the compositional changes of interest, or where the analytical quantities of interest were

non-chemical ones such as material properties or even sensory values ("taste") as determined by a test panel.

To understand the operation of NIRA and interpret its output more completely, it would be desirable to have available the spectra of the various sample constituents. These spectra could also be used to provide additional guidance for the multilinear regression. Unfortunately, the pure components are often unavailable and pure component spectra differ significantly from the spectra of samples perturbed by strong matrix effects.

Conveniently, the pure component spectra are implicitly generated during the multilinear regression. It should therefore be possible to extract from the regression the desired information and to display the reconstructed spectrum of the component of interest or of the property being investigated. In this operation, one inverts the common procedure of determining the composition of unknowns through use of reference spectra of the components, and instead generates these "reference spectra" from knowledge of the sample's quantitative composition.

In this paper, a rapid, convenient method for reconstructing near-infrared component spectra is introduced and evaluated. Based on a mathematical cross-correlation procedure, the technique requires only a set of near-infrared spectra of samples in which the concentration of the component of interest is known. From the correlation between those concentration values and the absorbance or reflectance of each sample at individual wavelengths, the spectrum of the individual constituent can be computed. Importantly, such spectra reflect the presence of the components in a particular sample and can be used to deduce the nature of matrix interactions. The new spectral reconstruction method is compared to other techniques of feature extraction and its extension to other spectral regions is considered.

I. THEORY

The key to this new method for spectral reconstruction is the use of mathematical cross-correlation.[5,6] From the simplest standpoint, cross-correlation evaluates the similarity between two waveforms, perhaps a sample and a reference. During this evaluation, cross correlation effectively recognizes and extracts those frequencies which are phase-registered in the sample and reference waveforms (ideally the signal) and eliminates all incoherent frequency components (noise).

This signal processing technique can be directly applied to the reconstruction of the spectrum of a desired component in a complex mixture. In this application, the sequence of absorbance values obtained for a series of mixtures at a particular wavelength comprises the sample "waveform". The sequence of concentrations of the desired component in that same series of mixtures then constitutes the reference "waveform". Cross-correlation of these two waveforms retains the signal (absorbance attributable to the desired component) and eliminates the noise (absorbance or background from any other source). When this process is repeated at a number of wavelengths over a selected range, the absorbance spectrum of the desired component is obtained.

In its most general form the cross-correlation function can be written as the discrete summation:

$$C_{ab}(d) = \frac{1}{n} \sum_{n} a(x)\ b(x \pm d) \qquad d = 0,1,2 \ldots n-1 \qquad (1)$$

where n is the number of samples, x is the sample index and d is the displacement from the current x index. $C_{ab}(d)$ is the value of cross-correlation function between signals a(x) and b(x) at the displacement d.

In the application of Eq. 1 to NIRA, a(x) is the absorbance (or its reflectance analog) of the xth sample at a specific wavelength and b(x) is the concentration of the desired component in the xth sample. In the absence of noise or other absorbing components in the sample set, the value of $C_{ab}(d)$ at $d = 0$ depends only on the absorbance and concentration of the desired component and all values of the cross-correlation function at $d \neq 0$ are zero. Clearly, in such a situation, it would be trivial to extract the desired spectrum from repeated applications of Eq. 1 at various wavelengths. In real samples, however, experimental noise sources, the interference of other sample constituents, and a limited number of samples cause the $d = 0$ and $d \neq 0$ terms of the cross-correlation function to contain small undesired contributions. To overcome these errors, the average of the $d \neq 0$ terms is subtracted from the value of $C_{ab}(d)$ at $d = 0$.[8] This correction is shown in Eq. 2.

$$C_{ab} = \frac{1}{n} \sum_{x=1}^{n} a(x)\ b(x) - \frac{1}{n(n-1)} \sum_{d=1}^{N-1} \sum_{x=1}^{n} a(x)\ b(x+d) \qquad (2)$$

Eq. 2 can be rewritten as:

$$C_{ab} = \frac{1}{n} \sum_{n} [a(x) - \bar{a}]\ [b(x) - \bar{b}] \qquad (3)$$

When this calculation is repeated for a number of wavelengths and plotted <u>vs</u> wavelength, the resulting spectrum shows the correlation between the sample absorbance and the concentration of the sought-for constituent and should be free of contributions from unwanted sources. The spectrum should therefore be that of the desired component.

When Eq. 3 is applied to a solution of non-interacting solutes, the concentration of each solute has no effect on the concentrations of the

others. Therefore, it is a simple matter to normalize Eq. 3 so the resulting reconstructed spectrum appears in convenient, concentration-independent units. This normalization can be effected by dividing Eq. 3 by the variance of b(x), as shown in Eq. 4.

$$C'_{ab} = \frac{\sum_{n} [a(x) - \bar{a}]\ [b(x) - \bar{b}]}{\sum_{n} [b(x) - \bar{b}]^2} \qquad (4)$$

A dimensional analysis of Eq. 4 shows that C'_{ab} has units of absorbance (concentration)$^{-1}$. Interestingly, if concentration (b) in Eq. 4 is expressed in fractional, dimensionless terms (e.g. weight fraction or mole fraction), the reconstructed spectrum that results from application of Eq. 4 has an amplitude corresponding to that of the pure component spectrum (where the fraction = 1).

In contrast to the above situation, some samples (especially solids) are comprised of mixtures where the fractional concentration of each species influences the others just because the fractional concentrations must sum to unity. Because of this interdependence, C'_{ab} (calculated from Eq. 4 as it is stated) which contain not only a correlation attributable to the desired component, but also a negative correlation caused by the effect of the concentration of that component on the concentrations of all other constituents.

To make a correction to Eq. 4 for this negative correlation it is necessary to express the concentration (b) of Eq. 4 in terms of weight fraction. As has been previously stated, this adjustment will produce a reconstructed spectrum representing a fractional concentration of 1. If there are negatively correlating species present, Eq. 4 will also scale

these negative correlations to those of the pure components (a fractional concentration of 1). With this information it then becomes possible to compute from each value of C'_{ab} in Eq. (4) the correct, normalized absorbance of the desired constituent.

The average absorbance of all samples at a particular wavelength ($\bar{a}$) can be viewed as the absorbance attributable to the desired pure component times its fractional concentration ($\bar{b}$) plus the average absorbance (at that wavelength) of all other species times their average fractional concentration ($1-\bar{b}$). In turn, the component in Eq. 4 caused by the previously discussed negative correlation is just the negative of the average absorbance (at that wavelength) of all species other than the desired one, scaled to a fractional concentration of unity. Accordingly, the negative correlation in Eq. (4) can be eliminated by scaling Eq. 4 to the true average concentration of "other" species [multiplying Eq. 4 by ($1-\bar{b}$)] and adding to the product the average sample absorbance at that wavelength ($\bar{a}$). In this procedure the positive correlation in Eq. 4 remains scaled to a fractional concentration of unity since the decrease caused by multiplying Eq. 4 by ($1-\bar{b}$) is exactly offset by the addition of $\bar{a}$ which has a fractional concentration of $\bar{b}$ of the desired constituent. This correction is shown in Eq. (5), an expression which is valid as long as the concentration [b(x) is expressed as a dimensionless fraction.

$$C''_{ab} = \left[\frac{\sum_n [a(x) - \bar{a}]\ [b(x) - \bar{b}]}{\sum_n [b(x) - \bar{b}]^2} \right] \left(1 - \bar{b}\right) + \bar{a} \qquad (5)$$

Of course, because correlation methods rely on linearity, Eqs. 3-5 will apply only in the absence of nonlinear effects such as physical or chemical nonadditivity (Beer's law deviations). Fortunately, this limitation is not

severe, because NIRA is also based on linear-response assumptions. Accordingly, a spectrum reconstructed by this new approach will be valid in all cases where NIRA is a useful technique.

II. EXPERIMENTAL

A. **Hydrocarbon mixtures.** Reagent-grade benzene (Mallinckrodt) and cyclohexane (MC&B), and spectranalyzed iso-octane and n-heptane (Fisher) were combined in varying proportions to create 97 standard hydrocarbon solutions. These solutions ranged from 3% to 100% concentration for each hydrocarbon. To minimize error, each of the four hydrocarbons was rapidly introduced and weighed by difference into a gas-tight vial. The error in each standard concentration is estimated at 0.05%. This value was obtained by propagation of an estimated error in weighing of 0.01 g. The volatility of the hydrocarbons and not the balance accuracy was the limiting factor in assessing this weighing error. Infrared spectra were recorded by a Digilab FTS-15C Fourier-transform spectrometer equipped with a silicon beam splitter, a PbSe detector operated at 300°C, and a CaF_2 flow-through cell. The instrumental resolution was nominally 4 cm^{-1} and boxcar apodization was employed.

B. **Protein and Moisture in Wheat.** A set of 50 near-infrared diffuse-reflectance spectra of wheat-flour samples was obtained from USDA, Beltsville, MD. Each of these spectra is comprised of 125 reflectance values obtained over the spectral range 1000-2587.2 nm in increments of 12.8 nm. The reported instrumental bandpass was 7 nm. Each of the flour samples was characterized for protein by 32 separate Kjeldahl measurements. Additional information on the data set has been published.[2] A spectrum of distilled

water was obtained from a 0.5 mm transmission cell with CaF_2 windows using the Digilab FTS-15C instrument described above.

Reconstructed spectra were calculated using a Data General Nova 3 computer. A FORTRAN program was written which interacts with Digilab-supplied software to access the individual sample spectra and generate the reconstructed spectrum. This program uses Eq. 5 exclusively in calculating the reconstructed spectrum.

III. RESULTS AND DISCUSSION

A. **Reconstructed Spectra.** The reconstructed spectrum of cyclohexane obtained from the hydrocarbon mixture is shown in Fig. 1 along with a spectrum of pure cyclohexane obtained during an independent run. A spectrum of a typical hydrocarbon mixture (benzene, cyclohexane, iso-octane and n-heptane) is shown in Fig. 2. A comparison of the reconstructed spectrum and that of the mixture shows that even intense background features in the mixture do not "bleed" through the reconstruction process and affect its accuracy. Moreover, the similarity of the values of the vertical scales in Fig. 1 shows the fidelity of the reconstructed spectrum; both the band location and amplitude are the same as found in the spectrum of the pure compound. Figures 3-5 show the pure and reconstructed spectra of the remaining components in the hydrocarbon mixtures. With the exception of a few small differences, each of these components show the same high degree of similarity between the pure and reconstructed spectra as found for cyclohexane. This similarity is not surprising; the compounds used to create the hydrocarbon mixture are known to exhibit few intermolecular interactions.

Although the reconstructed spectra of Fig. 1 and Figs. 3-5 appear very similar to those of the pure compounds, the spectra of the pure components were not used or required to generate the reconstructed spectra. Similarly,

the spectral reconstruction technique is able to produce spectra of individual mixture-components even when the pure components cannot be obtained. An example of this capability can be found in the determination of moisture in wheat flour.

An absorbance spectrum of pure water and the reconstructed spectrum of moisture in wheat flour, shown in Fig. 6, are noticeably different. In particular, the bands at 1.45 μm and 1.95 μm appear broader in the reconstructed spectrum than in the spectrum of pure water. This change is indicative of variations in hydrogen bonding caused by the protein matrix. Additionally, two small peaks at 2.15 μm and 2.3 μm appear in the reconstructed spectrum. These absorptions are due to protein and oil respectively and show that the moisture, protein and oil content of wheat are either biologically or chemically correlated.

As suggested earlier, the spectral reconstruction process should be able to extract from a sample set the composite spectrum of constituents responsible for sensory characteristics such as flavor or taste. A similar capability is the spectral reconstruction of Kjeldahl determined protein and "as is" protein.[2]

"As is" protein has been defined by Williams[2] as the protein value which has been determined by the Kjeldahl method but which has been adjusted for the moisture content of the sample. The reconstructed spectra of protein as determined by the Kjeldahl technique and by the "as is" measurement are reproduced in Fig. 7. These spectra are plotted on the same scale and are <u>not</u> offset. From Fig. 7, both measurements generate the same spectrum, suggesting that both measure essentially the same chemical species. However, there are some slight differences in the relative intensities of several of the peaks. For example, the moisture absorption band at 1.95 μm

is slightly smaller in the "as is" protein spectrum than in the Kjeldahl spectrum, indicating the "as is" measurement of protein reduces but does eliminate interferences from moisture.

B. **Comparison with Other Methods.** There are several alternative methods[9-12] which compete with the new spectral reconstruction scheme for extracting a spectrum from complex mixtures. Perhaps the most widely used of these techniques is spectral stripping or curve-fitting.[9]

Spectral stripping requires that the spectrum of all pure components be known and that the mixture be a linear combination of the pure components and not exhibit complicating interactions such as hydrogen bonding. These requirements are inconsistent with the characteristics of samples such as wheat or any others that contain interacting components. Changes in symmetry, chemisorption, physisorption and especially hydrogen bonding cause the spectra of most mixtures to be different from linear combinations of their components. In contrast, spectral reconstruction does not require pure component spectra and can deal with intermolecular interactions as shown in Fig. 6. Figure 6 shows a spectrum of reconstructed moisture in wheat which reasonably approximates pure water, but shows the spectral deviations of moisture in wheat described by Hruschka.[1]

A second method which can be used to generate data similar to the reconstructed spectrum is the ratio method.[10] This technique involves ratioing the spectra of several samples that contain the same components but in varying proportion. This ratio can then simply be used to locate regions of the spectrum where only one component absorbs. This method requires that each component must dominate the spectrum in at least one window region. According to Hirschfeld[10] the ratio method is valid only for relatively simple mixtures. Although the "simple mixtures" assumption might be true in the mid-infrared region, the broad and overlapping nature of the near-

infrared bands makes separating the spectra of even simple mixtures questionable. By comparison, the total number of species present in a sample affects spectral reconstruction only insofar as it increases the possible significance of random noise. Additional samples can be used to decrease the probability that random noise will have a significant contribution to the reconstructed spectrum.

A third method for decomposing spectral data is factor analysis.[11-13] The eigenvectors of factor analysis indeed provide spectral information on the discrete contributors present, and their eigenvalues are related to component concentrations. However, these eigenvectors represent only independently varying entities, and are not necessarily associated with specific (or indeed any) analytes. Even where such an association exists, it is not apparent, and its detection requires very good spectral differentiation, considerable expertise, or auxiliary chemical data. In the latter case, factor analysis can actually be complemented by an abridged form of spectral reconstruction. When the analyte sought contains independently varying components, that analyte will itself never appear as a factor, and its individual components might easily lie below the noise and be indetectable. In spectral reconstruction, on the other hand, the use of measured data drives the calculation to produce spectra corresponding precisely to the analyte of interest, even when the latter is ill-defined chemically, as seen in Fig. 6. In this example, factor analysis would separate the moisture, protein, oil and starch into separate eigenvectors whereas spectral reconstruction displays the proper combination of these components, and does so with an accurate indication of relative intensities.

Another difference between factor analysis and spectral reconstruction lies in how they treat noise. In factor analysis noise becomes a series of

factors, whose level sets a threshold for the smallest detectable real factor. In spectral reconstruction, each reconstructed spectrum will receive only that noise which is phase coherent with its analytical guiding values. All other noise appears as a residual when component spectra are substracted from the original data.

Spectral reconstruction is not without its drawbacks. Spectral reconstruction requires many more samples than does curve-fitting, and accurate reference chemical values which are not necessary for ratio deconvolution or factor analysis. However, NIRA applications also require several samples and accurate reference chemical values. This compatibility makes spectral reconstruction particularly well suited to elucidate the spectral details of NIRA samples and NIRA applications.

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FIGURE LEGENDS

1. Spectra of pure cyclohexane and one reconstructed from a mixture of cyclohexane, benzene, iso-octane and n-heptane. Scales have not been normalized.

2. Spectrum of a typical hydrocarbon standard composed of 12% benzene, 42% iso-octane, 26% cyclohexane and 20% n-heptane.

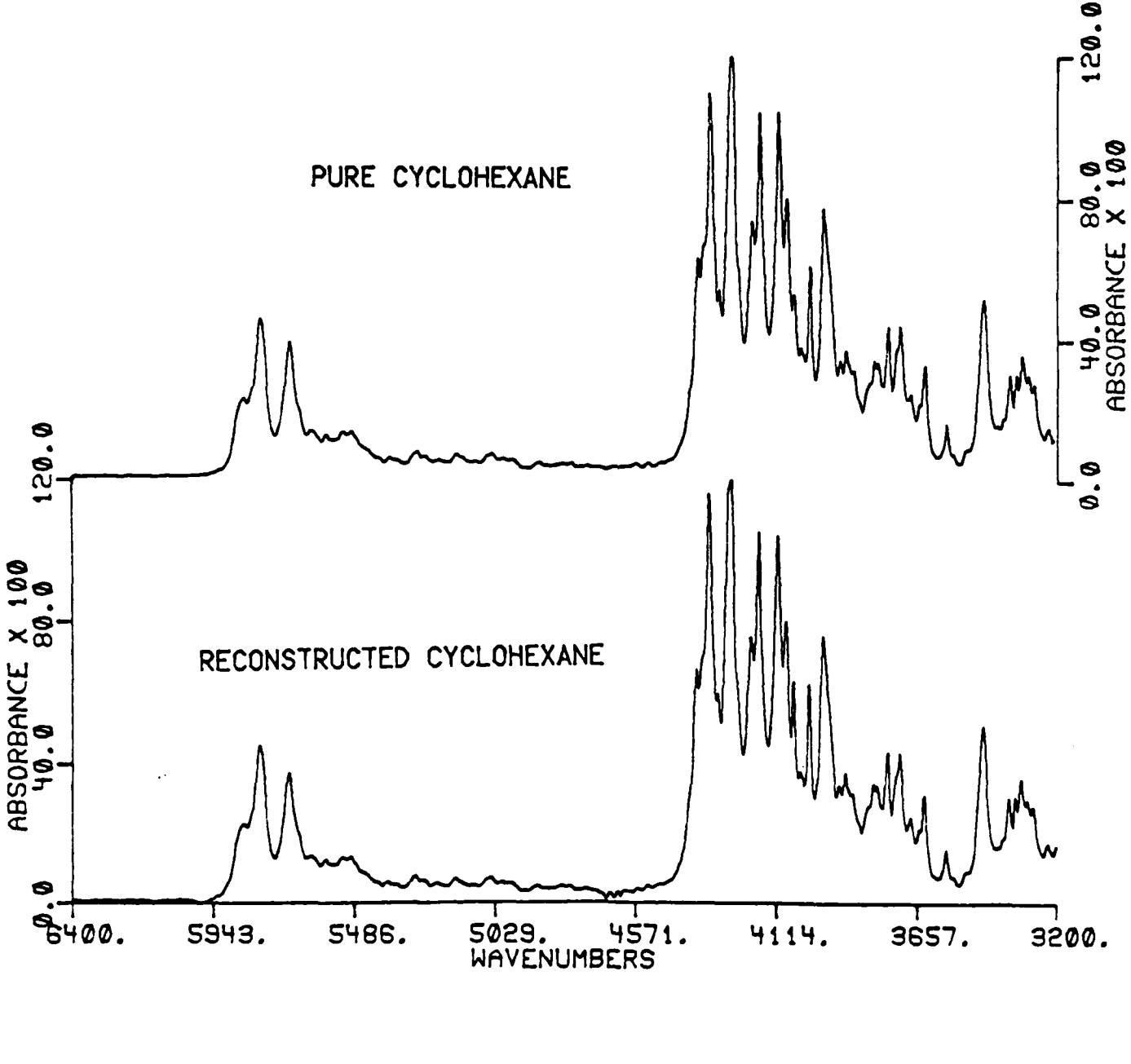
3. Spectrum of pure benzene and one reconstructed from hydrocarbon mixture. The peak at 4050 cm^{-1} has been clipped to enhance the smaller spectral structure.

4. Spectrum of pure n-heptane and one reconstructed from hydrocarbon mixture.

5. Spectrum of pure iso-octane and one reconstructed from hydrocarbon mixture.

6. Spectrum of pure H_2O and reconstructed spectrum of moisture in wheat.

7. Reconstructed spectra of Kjeldahl and "as is" protein determined in wheat.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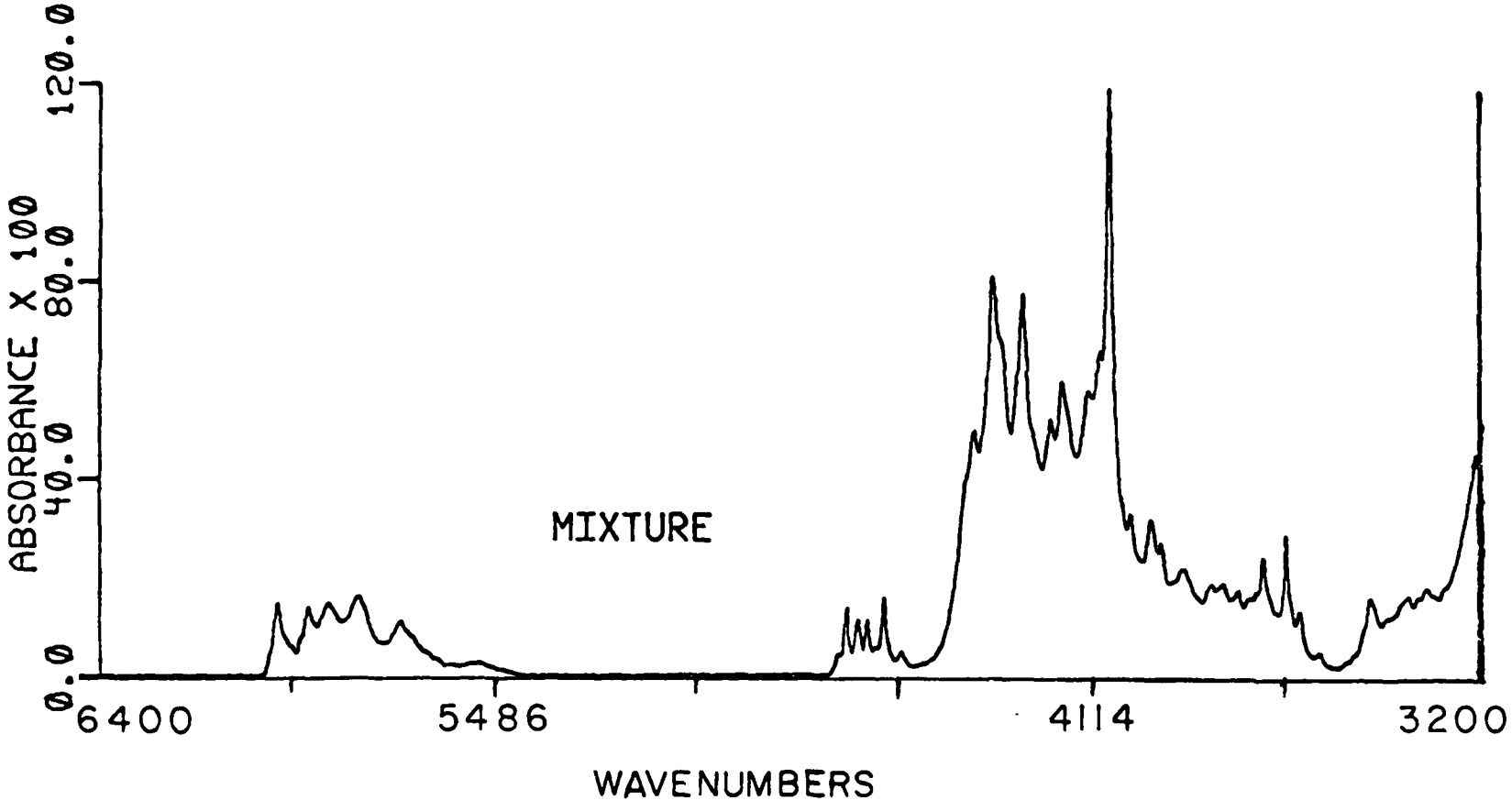
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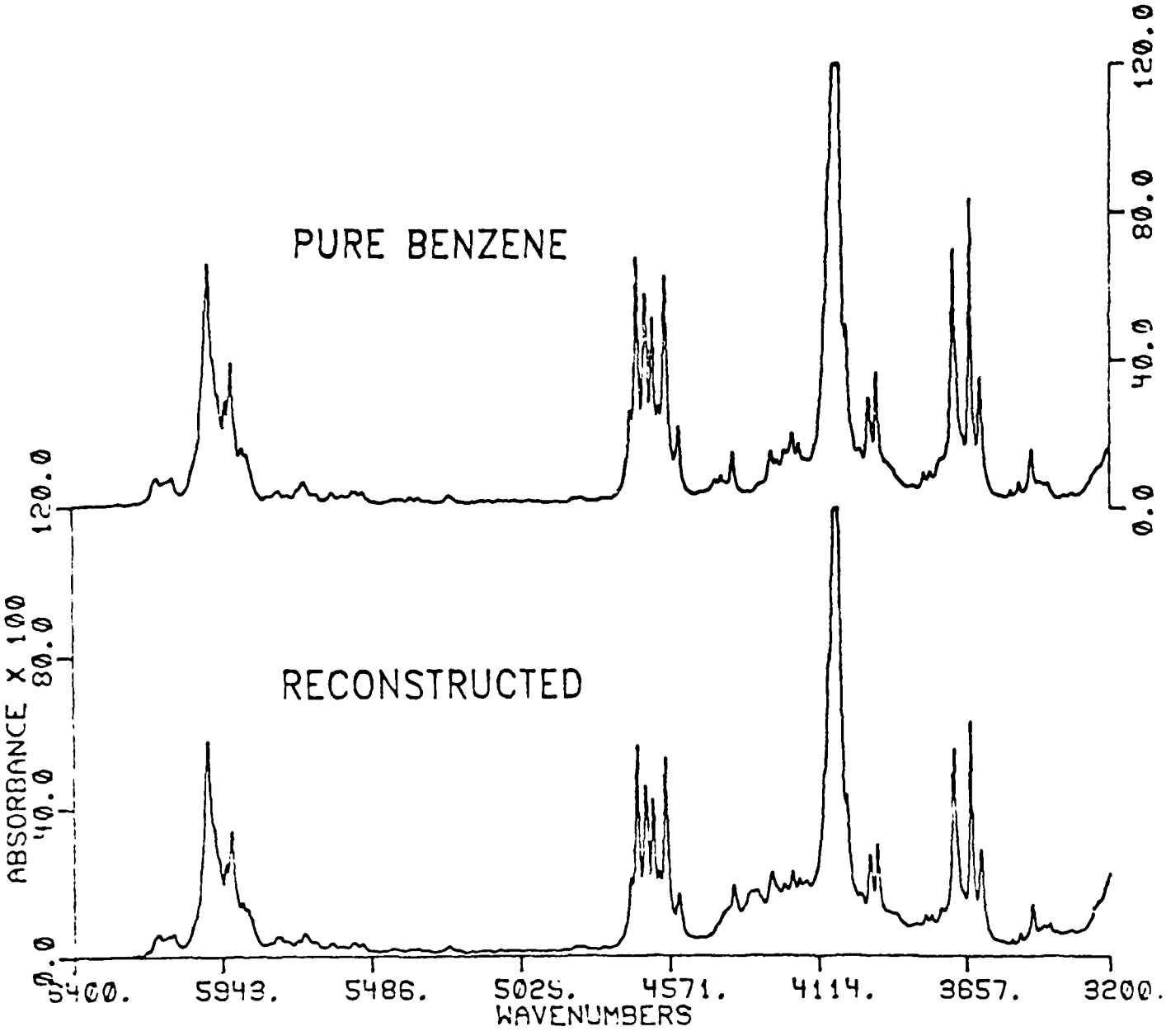
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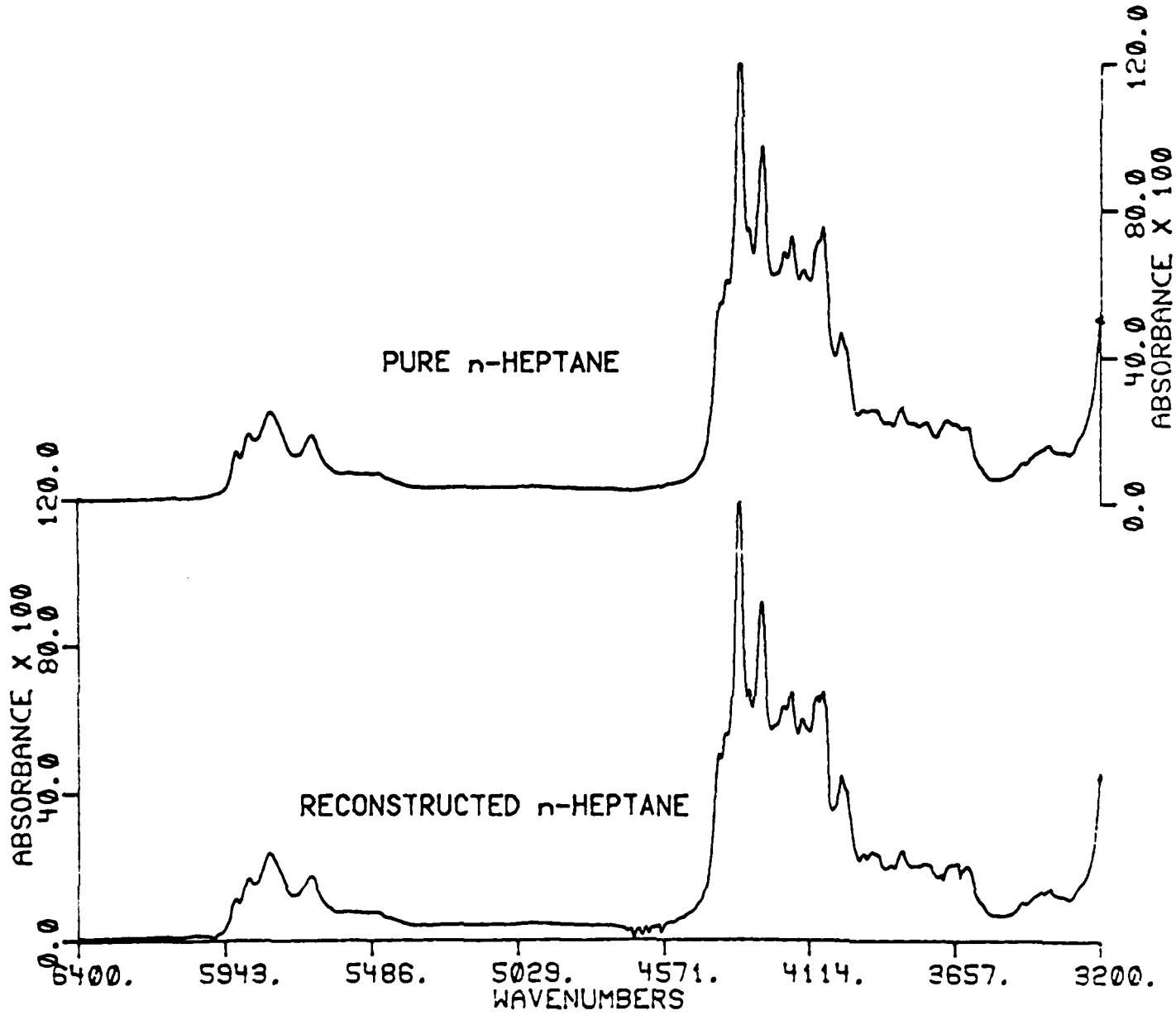
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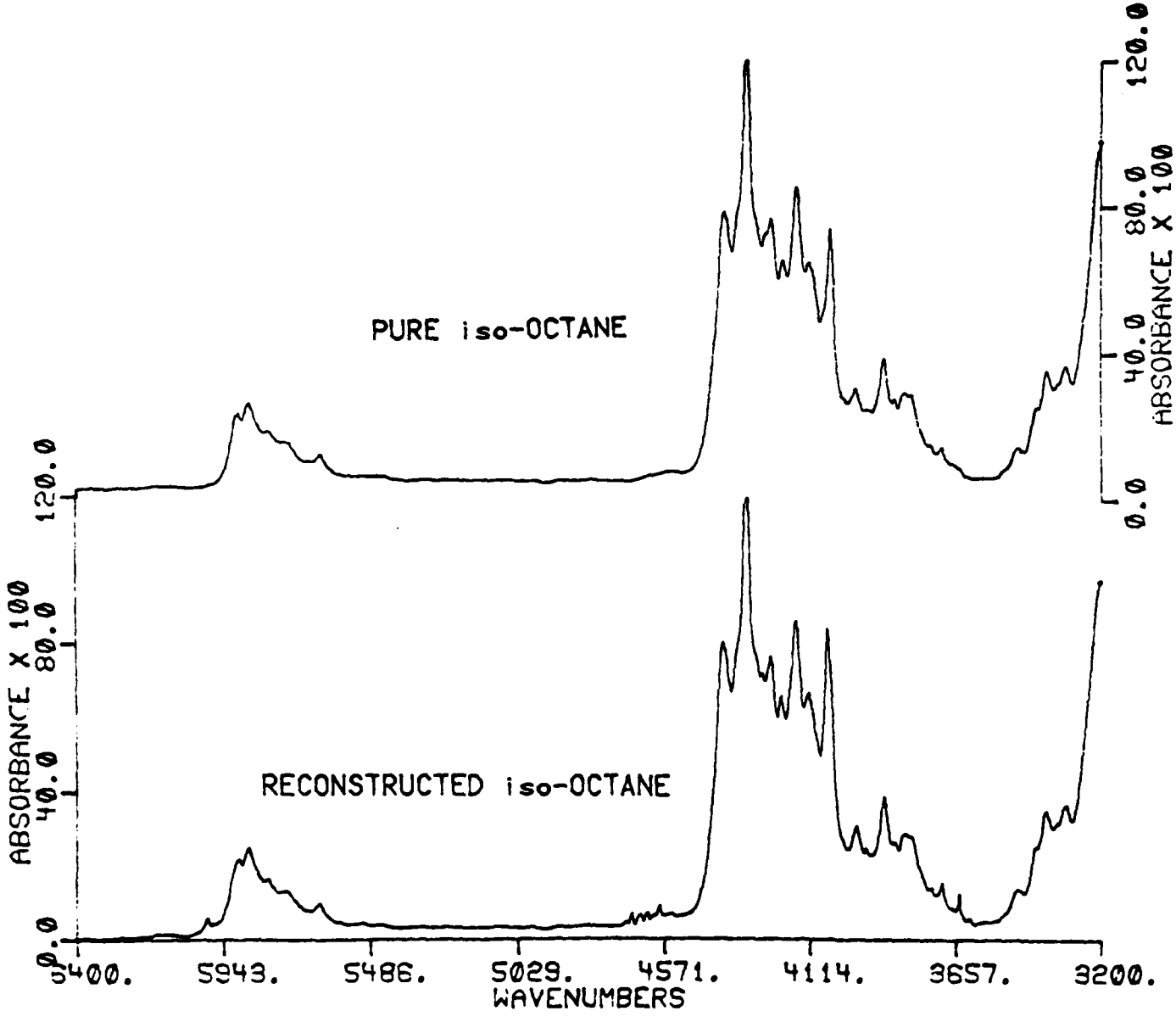
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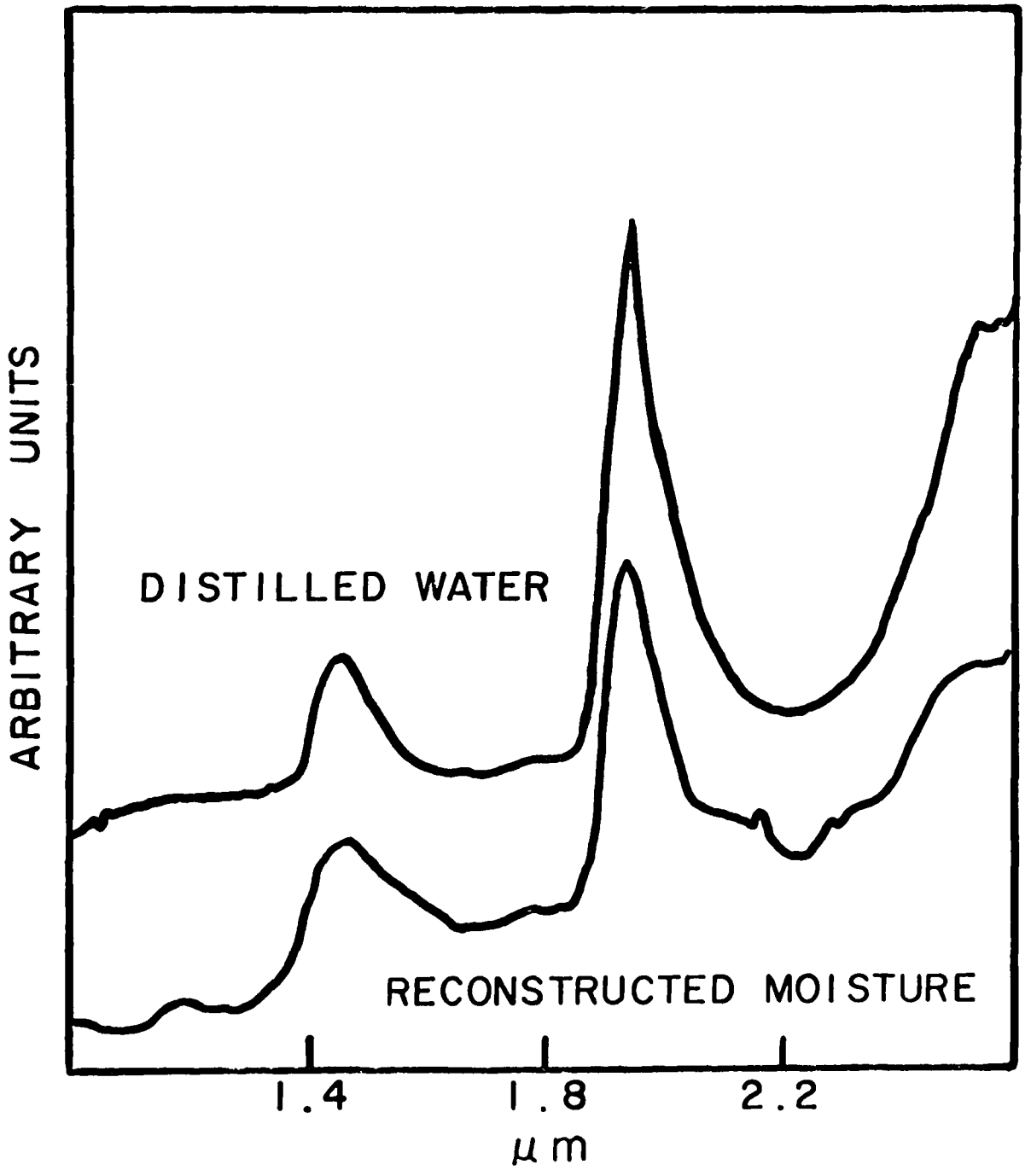
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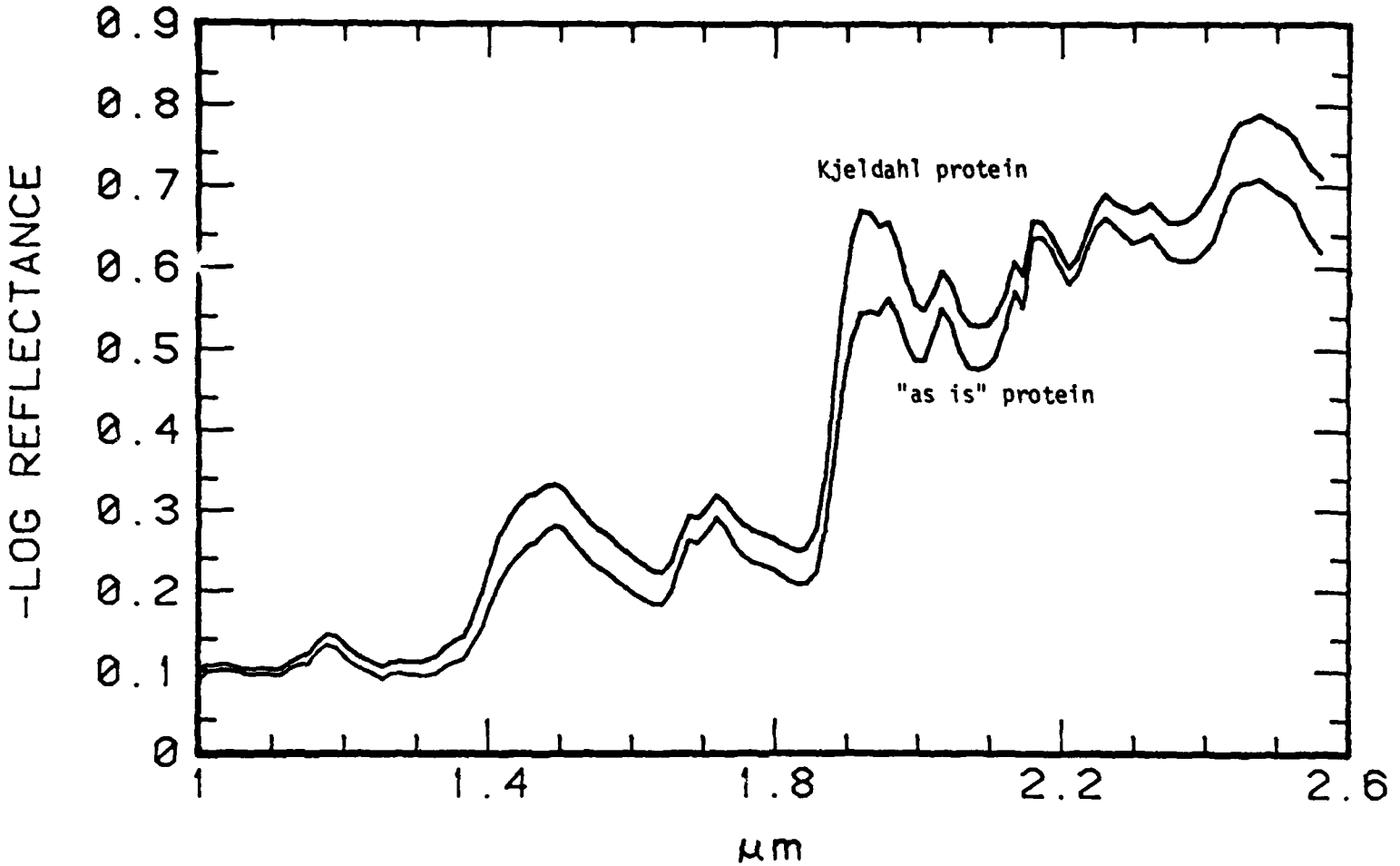
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